AFRL-AFOSR-VA-TR-2016-0333



Statistical inferences from the topology of complex networks

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10/11/2016 Final Report

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Final Report Statistical Inferences from the Topology of Complex Networks FA9550-13-1-0115

Awarded to PI: Peter Bubenik Current PI: John Holcomb

October 4, 2016

The project "Statistical Inferences from the Topology of Complex Networks" was funded by the AFOSR under the Complex Networks program, for the period March 1, 2013 to February 29, 2016. It was granted a No Cost Extension from March 1, 2016 to August 31, 2016. Here we offer a final report on the results of this project for the duration of the grant, from March 1, 2013 to August 31, 2016.

Change in PI

The project was awarded to Dr. Peter Bubenik at Cleveland State University. In August 2015, Dr. Bubenik moved to the University of Florida. Consequently, the PI on the project was changed to Dr. John Holcomb, the Chair of the Department of Mathematics at Cleveland State University. The remaining balance on the grant was sub-awarded to Dr. Bubenik at the University of Florida, where he continued to work on the project. All references to PI below are to Dr. Peter Bubenik.

Summary of the research

Main goals

As described in the abstract of the proposal for this project, its goals were "to develop and study a new topological descriptor that is designed for statistical

inference, and to use it for that purpose," and "to develop this topological machinery from a more abstract point of view, providing a better framework for studying its stability and for extending the scope of this technology."

Topological data analysis provides machinery for summarizing the topology of complex data as a "barcode" or "persistence diagram". While these have been successful tools for visualization, they are unsuitable for further statistical analysis or machine learning. The main goal of this project was to develop a new summary compatible with statistics and machine learning. This goal was met with the development of a new summary, the "persistence landscape". This summary is stable, does not lose any information, has continuous and discrete versions, and obeys a strong law of large numbers and a central limit theorem. The main results were published in the Journal of Machine Learning Research in a paper titled "Statistical topological data analysis using persistence landscapes" [4]. It is a functional summary which may be viewed as a point in a vector space (or more precisely, a point in a Hilbert space), and all of the standard tools in statistics and machine learning are available for subsequent analysis. For example, one can easily calculate averages and differences, and apply principal component analysis and support vector machines, or feed these results into a neural network.

The secondary goal of the project was to help place Topological Data Analysis on a firmer mathematical foundation, strengthening its connections to mathematics and making it easier for researchers to leverage mathematical results for analyzing complex data and complex networks. This goal was met with the publication of the paper (with J.A. Scott) "Categorification of persistent homology" [7] in the journal Discrete and Computational Geometry and the paper "Metrics for Generalized Persistence Modules" (with J.A. Scott and V. de Silva) in the journal Foundations of Computational Mathematics [5]. These papers develop a very general framework for topological data analysis.

Extensions of original goals

With the main goals achieved a number of extensions of these goals were pursued.

The topological summary, the "persistence landscape" developed in this project was validated by demonstrating that it could be combined with statistical inference and machine learning in a biological application. The resulting paper, "Using persistent homology and dynamical distances to analyze pro-

tein binding" (with V. Kovacev-Nikolic, D. Nikolic, and G. Heo) appeared in Statistical Applications in Genetics and Molecular Biology [18].

Together with P. Dlotko, the PI developed efficient algorithms for constructing the persistence landscape and for combining it with statistical analysis. The resulting article, "A persistence landscapes toolbox for topological statistics" is in the Journal of Symbolic Computation [6].

Together with P. Bendich, the PI has developed a framework and algorithm for stabilizing the location of topological features and also to stabilize topological computations with respect to choices of parameters. The paper "Stabilizing the output of persistent homology computations" has been submitted [3].

Together with V. de Silva and V. Nanda, the PI has studied the geometry of the algebraic objects of study in Topological Data Analysis. The resulting paper, "Higher interpolation and extension of persistence modules" is undergoing peer review.

Impact on the community

The main contribution of this project, the persistence landscape, is perhaps the most influential development in this research area in the past few years. The paper [4] has inspired considerable theoretical research and is starting to be used in a wide variety of applications. The bootstrap has been applied to provide confidence bands for the persistence landscape [11, 10]. The persistence landscape has also inspired a number of other linear topological summaries [11, 22, 8, 23, 1, 19, 12, 13, 25, 2]. The persistence landscape has been used to study brain images [24], fluid dynamics [16], brain EEG data [26], complex networks [9], and phase transitions [17]. It has also been recently combined with Neural Networks to study audio signals [20]. According to Google Scholar this paper has already been cited 70 times.

The secondary goal of the project was the development of a general framework for topological data analysis, which was given in [7] and [5]. This framework has already been used by other researchers to develop algorithms and prove properties in concrete settings such as those for Reeb graphs [14, 21]. According the Google Scholar these papers have 42 and 13 citations respectively.

Software development

The algorithms for persistence landscapes and statistical inference presented in [6] have been implemented as "The Persistence Landscape Toolbox" and the code is publicly available [15].

Dissemination of results

During this project the PI gave 26 invited lectures describing its results. The venues for these talks included research institutes and leading universities in the United States, Canada, Mexico, the United Kingdom, Germany, Denmark, Poland and Japan.

Broader impacts

The PI has made efforts to increase the broader impact of the project. He founded and serves as Director of the Applied Algebraic Topology Research Network, a network with close to 300 members that is funded by the NSF through the Institute of Mathematics and its Applications (IMA). He also accepted a position as Associate Editor at the new (Society for Industrial and Applied Mathematics) SIAM Journal on Applied Algebra and Geometry. In addition he was a member of the Scientific Committee for the main conference in this subject, "Applied Topology: Computation, Methods, and Science," held in Turin, Italy, in July 2016.

The PI has given outreach talks at the NASA Glenn Research Center's Summer Intern Seminar, and to the University of Florida Graduate Mathematics Association Colloquium. He was also the featured speaker at a Summer School organized by the Mathematical Association of America entitled "Big Data on the Great Plains."

At Cleveland State University and the University of Florida (UF) he has been using the results of this project to teach undergraduate and graduate students. At UF, he has incorporated TDA into the graduate topology course and he started a Student Applied Topology seminar.

At UF, the PI has also been training Highly Qualified Personnel. These will be future researchers and data analysts and this training will aid the competitiveness of the United States. He is advising one postdoctoral researcher, Dr. Michael Catanzaro, two Ph.D. candidates, Alexander Wagner

and Leo Betthauser, and two undergraduate students, Benjamin Whittle and Dhruv Patel.

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FA9550-13-1-0115

Principal Investigator Name

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Peter Bubenik

Program Officer

The AFOSR Program Officer currently assigned to the award

James Lawton

Reporting Period Start Date

03/01/2013

Reporting Period End Date

08/31/2016

Abstract

Topological data analysis provides machinery for summarizing the topology of complex data. The main goal of this project was to develop a new summary compatible with statistics and machine learning. This goal was met with the development of a new summary, the "persistence landscape." This summary is stable, does not lose any information, has continuous and discrete versions, and obeys a strong law of large numbers and a central limit theorem. All of the standard tools in statistics and machine learning are available for subsequent analysis. For example, one can easily calculate averages and differences, apply principal component analysis and support vector machines, or feed these results into a neural network. The secondary goal of the project was to help place Topological Data Analysis on a firmer mathematical foundation, strengthening its connections to mathematics and making it easier for researchers to leverage mathematical results for analyzing complex data and complex networks. This goal has been met with the development a very general framework for topological data analysis. Both of these developments have led to much work by other researchers.

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Peter Bubenik, Vin de Silva, and Jonathan Scott. Metrics for generalized persistence modules, Foundations of Computational Mathematics 15 (2015), no.6, 1501–1531.

Violeta Kovacev-Nikolic, Peter Bubenik, Dragan Nikolic, and Giseon Heo. Using persistent homology and dynamical distances to analyze protein binding, Statistical Applications in Genetics and Molecular Biology 15 (2016) no. 1, 19–38.

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